



chain nodes :

13 14 16 17 19 21 22 23 34 40 41 42 43 48

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 15 18 20 24 25 26 27 28 29 30 31 32 33 35 36
37 38 39

chain bonds :

9-48 13-14 13-34 14-15 16-17 17-18 19-20 21-22 21-43 22-23 23-40 40-41 40-42

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-11 7-8 8-9 9-10 10-11 15-24 15-28 18-29 18-33
20-35 20-39 24-25 25-26 26-27 27-28 29-30 30-31 31-32 32-33 35-36 36-37 37-38
38-39

exact/norm bonds :

4-7 5-11 7-8 8-9 9-10 9-48 10-11 15-24 15-28 18-29 18-33 20-35 20-39 22-23 23-40
24-25 25-26 26-27 27-28 29-30 30-31 31-32 32-33 35-36 36-37 37-38 38-39 40-41

exact bonds :

13-14 13-34 14-15 16-17 17-18 19-20 21-22 21-43 40-42

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

G1: [*1] , [*2] , [*3] , [*4]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
13:CLASS 14:CLASS 15:Atom 16:CLASS 17:CLASS 18:Atom 19:CLASS 20:Atom 21:CLASS 22:CLASS
23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom
33:Atom 34:CLASS 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:CLASS 41:CLASS 42:CLASS
43:CLASS 48:CLASS